N-(1-Naphthyl)ethylenediamine 551-09-7 | DTXSID7043744

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Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 9.11e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.95e-01

Confidence level: 4.10e-01

Nearest Neighbors from the Training Set

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1,10-Phenanthroline Measured: 1.49e-02 Predicted: 5.60e-03

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N-(1-Naphthyl)ethylenediamine

Measured: 1.07e-02 Predicted: 9.11e-02

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Nabam-sodium Measured: 7.80e-01 Predicted: 2.66e-01

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1-Phenyl-2-thiourea Measured: 1.62e-02 Predicted: 7.48e-02

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Quinoxaline Measured: 5.07 Predicted: 1.30e-01